Measures of Quantum State Purity and Classical Degree of Polarization

Omar Gamel* and Daniel F. V. James

Department of Physics, University of Toronto, 60 St. George St., Toronto, Ontario, Canada M5S 1A7.

There is a well known mathematical similarity between two dimensional classical polarization optics and two level quantum systems, where the Poincare and Bloch spheres are identical mathematical structures. This analogy implies classical degree of polarization and quantum purity are in fact the same quantity. We make extensive use of this analogy to analyze various measures of polarization for higher dimensions proposed in the literature, and in particular, the $N = 3$ case, illustrating interesting relationships that emerge as well the advantages of each measure. We also propose a possible new class of measures of entanglement based on purity of subsystems.

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I. INTRODUCTION

There exists a well known mathematical similarity between classical polarization optics in two dimensions and quantum two level systems. The Stokes vector and Poincare sphere on the one hand [1] are analogous to the Bloch vector and Bloch sphere on the other [2]. The Pancharatnam phase in classial optics systems [3] corresponds to the Berry phase in quantum systems [4].

Note that the point at the origin of the Poincare sphere represents a completely unpolarized beam of light, while any point on the surface of the sphere represents a completely polarized beam. In the case of the Bloch sphere, the origin represents the maximally mixed state while any point on the surface represents a pure state. This suggests an additional analogy between the two systems, that classical polarization is analogous to quantum purity, and measures of the two quantities should therefore be identical. This analogy between polarization and purity has been discussed by some authors for a particular measure of polarization in higher dimension [5].

In this paper, we start by discussing in more detail the analogy between the classical and quantum cases, followed by a review of classical polarization in two dimensions. We then move to higher dimensions, with particular attention to the three dimensional case. In doing so, we come across measures for quantum purity from quantum mechanics, namely the standard purity and von Neumann purity [6]. We also analyze measures of polarization in three dimensions due to Barakat [7], Friberg et. al. [8], and Wolf et al. [9]. We then proceed to compare these measures analytically, numerically and give them physical interpretations where possible. Our analysis adds to and clarifies much of the discussion on measures of higher dimensional polarization in the literature [10–14].

Furthermore, we point out that the entanglement of a bipartite pure state can be thought of as the purity / polarization of a subsystem is traced out. This suggests that using unconventional measures of purity, we can create new and interesting measures of entanglement.

*Electronic address: ogamel@physics.utoronto.ca

II. POLARIZATION OF BEAMS AND PURITY OF QUBITS

A. Classical polarization states

Consider a classical beam of light propagating in the z direction. Using the stochastic theory of electrodynamics, the magnitude of the electric field in the x and y direction are taken to be probabilistic ensembles given by E_1 and E_2 respectively [15, 17, 18]. The polarization state of the beam of light at any point is given by the 2×2 correlation matrix $\Gamma^{(2)}$, defined as follows,

$$\Gamma^{(2)}_{ij} = \langle E_i E_j^* \rangle, \qquad i = 1, 2 \tag{1}$$

where $\langle\rangle$ denotes the ensemble average over different possible realizations. We then define the polarization matrix Φ as the normalized Γ, that is

$$\Phi^{(2)} = \Gamma^{(2)} / \operatorname{Tr}[\Gamma^{(2)}]. \tag{2}$$

Therefore the polarization matrix $\Phi^{(2)}$ has unit trace by definition. In the following paragraphs, we suppress the dimensional superscript on the polarization matrix. Alternatively, the four normalized Stokes parameters, s_μ, can be used to represent the polarization state [1]. They are related to Φ as follows,

$$s_\mu = \operatorname{Tr}[\Phi \sigma^\mu] = \Phi_{ij} \sigma^\mu_{ji}, \tag{3}$$

$$\Phi = \frac{1}{2} s_\mu \sigma^\mu, \tag{4}$$

where σ^0 is the identity matrix, and σ^1, σ^2, and σ^3 are the three Pauli matrices σ^z, σ^x, and σ^y respectively. Einstein summation notation has been used, i.e. repeated indices are summed over. Lowercase Latin letters run from 1 to 2 (corresponding to the two Cartesian components of the field), while lowercase Greek letters run from 0 to 3. Since Φ is of unit trace, s_0 is always unity. It can be shown that Φ must be a positive matrix, which in turn

implies the following condition on the normalized Stokes parameters [20],

$$s_1^2 + s_2^2 + s_3^2 \leq s_0^2 = 1. \tag{5}$$

Immediately we see that eq.(9) becomes the equation of a unit sphere, and taken as a position vector s_1, s_2 and s_3 describe a point on or within a unit sphere, called the Poincare sphere. The degree of polarization, $P^{(2)}$ of a 2-dimensional polarization matrix Φ is derived by writing Φ as the unique sum of two polarization matrices, one completely unpolarized (i.e. a multiple of the identity), and one completely polarized [18]. The degree of polarization is then the ratio of "power" contained in the completely polarized matrix to the total power. It is given by,

$$P^{(2)} = \sqrt{1 - 4\det(\Phi)}. \tag{6}$$

Using eq.(4) to write eq.(6) in terms of the Stokes parameters, we find that the degree of polarization is,

$$P^{(2)} = \sqrt{s_1^2 + s_2^2 + s_3^2}. \tag{7}$$

That is, the degree of polarization is simply the distance from the origin of the Stokes vector within the normalized Poincare sphere. This makes intuitive sense and is a natural measurement, since the origin (where $P^{(2)} = 0$) represents the completely unpolarized state, and the surface of the sphere (where $P^{(2)} = 1$) represents the set of completely polarized states, and the value of P for other states is "linear" in the distance metric within the Poincare sphere.

B. Quantum two level system

The most general quantum state is expressed in terms of the density matrix ρ, which contains all the statistically observable information of the state. This matrix is positive, Hermitian, and of unit trace. In the case of a qubit, it is of dimension 2×2. We can write ρ as a linear combination of the identity and Pauli matrices as follows [6],

$$\rho = \frac{1}{2}(I + r_1\sigma_1 + r_2\sigma_2 + r_3\sigma_3), \tag{8}$$

where $\vec{r} = (r_1, r_2, r_3)$ is the well-known Bloch vector [2]. Note that eq.(8) is in fact identical to eq.(4). Moreover, since ρ is positive, we can also show that,

$$r_1^2 + r_2^2 + r_3^2 \leq 1. \tag{9}$$

Therefore, the Bloch vector also lies within a unit sphere, known as the Bloch sphere. It is clear that in the 2-dimensional case, the quantum density matrix ρ is analogous to the classical polarization matrix Φ, and that the Bloch sphere is analogous to the Poincare sphere, since they have an identical mathematical structure. We also see that the state at the origin of the Bloch sphere is the maximally mixed state whereas states on the surface of the sphere are pure states. Comparing this with the Poincare sphere, where the origin is a completely unpolarized state and the surface contains completely polarized states, this suggests a direct analogue between quantum purity and and classical degree of polarization. Therefore, measures of the two quantities are for most purposes equivalent, and we keep this in mind in what follows.

III. MEASURES OF PURITY AND POLARIZATION FOR N DIMENSIONS

We proceed to introduce various measures of purity / polarization that have been suggested in the quantum mechanics and classical optics literature. Since purity is a property intrinsic to the density operator and invariant of the basis used, it should be invariant under unitary transformations. Therefore, one can always choose the basis where the density matrix is diagonal, and therefore, purity should be expressible as a function of the eigenvalues of ρ alone, which we write as $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_N$, for an N dimensional system.

If we write the purity as function of the eigenvalues, denoted by $\Pi(\lambda_1, ..., \lambda_N)$, then we require that it be a real-valued function that is scaled such that it takes values between 0 and 1. It should take value 1 for a pure state and 0 for the maximally mixed state; that is, $\Pi(1, 0, ..., 0) = 1$ and $\Pi(1/N, 1/N, ..., 1/N) = 0$, respectively.

A. Standard purity

In quantum information science, the common measure of purity for a quantum state ρ in an N dimensional system is given by $\mathrm{Tr}[\rho^2]$ [6]. It takes a maximum value of 1 for a pure state, and minimum value of $\frac{1}{N}$ for the maximally mixed state. This purity is often scaled linearly so it varies between 0 and 1, giving the following expression, which we call standard purity,

$$\Pi_s(\rho) \equiv \frac{N\,\mathrm{Tr}[\rho^2] - 1}{N - 1}. \tag{10}$$

In terms of eigenvalues,

$$\Pi_s(\rho) = \frac{N\sum_{i=1}^{N}\lambda_i^2 - 1}{N - 1}. \tag{11}$$

B. Von Neumann purity

Shannon entropy is used in classical systems to quantify uncertainty about a random variable. Von Neumann entropy generalizes this to quantum systems, and is given by,

$$S(\rho) \equiv -\mathrm{Tr}[\rho\log_2(\rho)]. \tag{12}$$

This measure quantifies the departure of a state from a pure state, i.e. its "mixedness" [6]. Note that the entropy of entanglement (a popular measure of entanglement for bipartite pure states) is defined to be the von Neumann entropy of one of the subsystems when the other subsystem is traced out. This implies that the von Neumann entropy is a good measure of mixedness. Therefore, one can define another measure of purity, $\Pi_v(\rho) \in [0,1]$, based on the von Neumann entropy,

$$\Pi_v(\rho) \equiv 1 + \frac{\mathrm{Tr}[\rho \log_2(\rho)]}{\log_2 N} \tag{13}$$

Expressed as a function of eigenvalues, von Neumann purity is given by,

$$\Pi_v(\rho) = 1 + \frac{1}{\log_2 N} \sum_{i=1}^{N} \lambda_i \log_2(\lambda_i). \tag{14}$$

C. Polarization purity for N=2

For the simple case of the two dimensional system, we have already seen that the classical degree of polarization is given by eq.(6). Therefore, we have the *two dimensional polarization purity* given by $P^{(2)}$, defined as,

$$P^{(2)}(\rho) \equiv \sqrt{1 - 4\det(\rho)}. \tag{15}$$

In terms of the two eigenvalues of ρ, this can be written as,

$$\begin{aligned} P^{(2)}(\lambda_1, \lambda_2) &= \sqrt{1 - 4\lambda_1\lambda_2} \\ &= \lambda_1 - \lambda_2, \end{aligned} \tag{16}$$

where in the last equality, we used the fact that $1 = (\lambda_1 + \lambda_2)^2$. Moreover, as pointed out in the classical polarization case, $P^{(2)}$ is simply the length of Bloch vector that represents ρ. That is, if we express the density matrix ρ as a Bloch vector as in eq.(8), we find that polarization purity simplifies to,

$$P^{(2)}(\vec{r}) = \sqrt{r_1^2 + r_2^2 + r_3^2} = |\vec{r}|. \tag{17}$$

We wish to generalize polarization purity $P^{(2)}$ to $N > 2$ dimensions. Obviously, in principle there are an infinite number of ways to do this. However, only a handful of them have physical significance. In the following subsections, we discuss three possible generalizations that naturally follow from eqs. (15), (16), and (17) respectively. In particular, we pay particular attention to the $N = 3$ case, since it corresponds to classical polarization in three dimensions, a problem about which there is no consensus as of yet.

D. Barakat heirarchy measures of purity

In the case of an $N \times N$ density matrix ρ, Barakat has introduced a hierarchy of $N - 1$ purity measures [7]. These measures are defined by first writing out the characteristic polynomial equation of ρ as follows,

$$\begin{aligned} \det(\rho - \lambda\mathbb{I}) &= \lambda^N - C_1\lambda^{N-1} + C_2\lambda^{N-2} - ... + (-1)^N C_n \\ &= 0. \end{aligned} \tag{18}$$

The roots of this polynomial equation are clearly the eigenvalues of ρ (by definition). Each coefficient C_k is the sum of all possible unique products of k eigenvalues of ρ. That is,

$$C_k = \sum_{1 \le i_1 \le \ldots i_k \le N} \prod_{j=1}^{k} \lambda_{i_j}. \tag{19}$$

For example, if $N = 3$, then,

$$\begin{aligned} C_1 &= \lambda_1 + \lambda_2 + \lambda_3 = 1, \\ C_2 &= \lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3, \\ C_3 &= \lambda_1\lambda_2\lambda_3 = \det(\rho). \end{aligned} \tag{20}$$

In fact $C_1 = 1$ and $C_N = \det(\rho)$ both hold for any N. Moreover, it can be shown that each C_k is expressible in terms of $\mathrm{Tr}(\rho^m)$, for $m = 2, ...k$, or alternatively in terms of the first k Casimir invariants of ρ [23, 24]. For example, for any N, we have,

$$C_2 = [1 - \mathrm{Tr}(\rho^2)]/2, \tag{21}$$

$$C_3 = [1 - 3\,\mathrm{Tr}(\rho^2) + 2\,\mathrm{Tr}(\rho^3)]/6. \tag{22}$$

Therefore, the C_k are invariant under change of coordinates. If ρ is a pure state (i.e. has rank 1), then all the C_k are zero, except for C_1 which is always unity. If ρ is the maximally mixed state (all eigenvalues are $\frac{1}{N}$), then $C_k = \binom{N}{k}\frac{1}{N^k}$ where $\binom{N}{k}$ is the binomial coefficient.

With this in mind and noting that C_k coefficients themselves can be thought of as a measure of purity, Barakat then defines a hierarchy of measures of polarization given by $B_k^{(N)}(\rho)$ for $k = 2, ...N$. Requiring that $B_2^{(2)}(\rho)$ collapse to $P^{(2)}(\rho)$ in eq.(15), one defines,

$$B_k^{(N)}(\rho) \equiv \sqrt{1 - \binom{N}{k}^{-1} N^k C_k}, \quad k = 2, ..., N, \tag{23}$$

The measure $B_k^{(N)}(\rho)$ takes the value zero for all k in the maximally mixed (i.e. the fully unpolarized) state, and takes the value 1 for all k when ρ is a pure (fully polarized) state. To get a feel for these measures, let us explore and simplify them using eq.(22) for some specific values of N and k. For $N = 2$, we have

$$B_2^{(2)}(\rho) = \sqrt{1 - 4\det(\rho)} = P^{(2)}(\rho), \tag{24}$$

as we required. For $N = 3$ we have,

$$B_2^{(3)}(\rho) = \sqrt{\left[3\,\mathrm{Tr}(\rho^2) - 1\right]/2}, \tag{25}$$

$$\begin{aligned} B_3^{(3)}(\rho) &= \sqrt{1 - 27\det(\rho)}, \\ &= \sqrt{1 - 27\lambda_1\lambda_2\lambda_3}. \end{aligned} \tag{26}$$

For general N we have,

$$B_2^{(N)}(\rho) = \sqrt{\frac{N\,\mathrm{Tr}(\rho^2)-1}{N-1}} = \sqrt{\Pi_s(\rho)}, \tag{27}$$

$$\begin{aligned} B_N^{(N)}(\rho) &= \sqrt{1-N^N \det(\rho)}, \\ &= \sqrt{1-N^N \lambda_1\lambda_2...\lambda_N}. \end{aligned} \tag{28}$$

Note the interesting relationship in eq.(27) where $B_2^{(N)}$ is simply the square root of the standard measure of purity Π_s. However, $B_N^{(N)}$ is unique, therefore we define *Barakat's last measure* of purity as Π_b, given by,

$$\Pi_b(\rho) \equiv B_N^{(N)}(\rho). \tag{29}$$

We add Π_b to our collection of measures which will be compared to other measures later in this paper.

E. KW purity

Another measurement of 3-dimensional polarization proposed by Korotkova and Wolf relies on the total power in the completely polarized component [9, 10]. That is, one splits the 3×3 polarization/density matrix into a unique positive linear combination of the identity matrix, a rank 2 matrix with degenerate eigenvalues, and a rank 1 matrix. The degree of polarization, Π_{kw} is defined to be the coefficient of the (fully polarized) rank 1 matrix. We call this measure, the *KW purity.* It is given by,

$$\Pi_{kw}(\rho) = \lambda_1 - \lambda_2. \tag{30}$$

This is identical to *eq.*(16) in two dimensions. In fact, this particular measure has the same form for any $N \geq 2$, it is always the difference between the largest two eigenvalues. The advantage of this measure is that it is very physically meaningful. It is the fraction of the power that can be rendered into a completely polarized field by passive linear elements. That is, if we use some (hypothetical) 3-dimensional polarizers, we should be able to extract the power of this fully polarized component.

However, when one considers the rank 2 component of the polarization matrix (when broken up as we discussed two paragraphs above), one sees that this component is not fully polarized, but neither is it fully unpolarized. This suggests that it should have some intermediate polarization of its own, and make a contribution to the level of polarization of the density matrix. Since Π_{kw} ignores the rank 2 component completely, this suggests it is not well suited for as a measure of overall polarization, but is rather suited for measuring only the component of a field that is completely polarized. We clarify this in the next section with an illustrative example.

F. SSKF purity

There have been multiple suggested measures of three-dimensional polarization [8–10], which rather than dealing with a beam propagating in one direction, deals with an arbitrary electric field distribution in 3 dimensions. The measure due to Setälä, Shevchenko, Kaivola, and Friberg [8] starts by writing an equation similar to eq.(8), to decompose the 3×3 density matrix ρ. It is,

$$\rho = \frac{1}{3}\mathbb{I} + \frac{1}{\sqrt{3}}\sum_{i=1}^{8} r_i \hat{G}_i, \tag{31}$$

where $\mathbb{I}$ is the identity, and $\hat{G}_i, i = 1-8$ are a popular 3 dimensional analogue of the Pauli matrices, known the Gell-Mann matrices [22], shown in the first Appendix. We have modified the coefficients from the Friberg paper to ease calculation. The eight coefficients r_i together form a (generalized) Bloch vector $\vec{r}$. One can use eq.(31) together with the orthogonality and tracelessness of Gell-Mann matrices to show that,

$$\mathrm{Tr}\,[\rho^2] = \frac{1}{3} + \frac{2}{3}|\vec{r}|^2. \tag{32}$$

The density matrix condition $\mathrm{Tr}\,[\rho^2] \leq 1$ implies that $\sum_{i=1}^{8} r_i^2 = |\vec{r}|^2 \leq 1$, that is the Bloch vector $\vec{r}$ lies inside an 8-dimensional hypersphere of unit radius. The polarization is then defined in a manner analogous to eq.(7) and eq.(17) as the length of the Bloch vector, i.e. the radial distance from the origin in this hypersphere, given by,

$$\Pi_{sskf}(\rho) \equiv \Big[\sum_{i=1}^{8} r_i^2\Big]^{\frac{1}{2}} = |\vec{r}|. \tag{33}$$

We call this the *SSKF purity* or the radial purity, emphasizing that it gives the length of a radial Bloch vector in a hypersphere. Equivalently, one can also invert eq.(32) to write the SSKF purity as a direct function of ρ,

$$\Pi_{sskf}(\rho) = \sqrt{\big[3\,\mathrm{Tr}(\rho^2) - 1\big]/2}, \tag{34}$$

or its eigenvalues λ_1, λ_2, and λ_3,

$$\Pi_{sskf}(\rho) = \sqrt{\frac{1}{2}\Big[3(\lambda_1^2 + \lambda_2^2 + \lambda_3^2) - 1\Big]}. \tag{35}$$

Note that the equation above is identical to eq.(25), and therefore $\Pi_{sskf}(\rho) \equiv B_2^{(3)}(\rho)$ for $N = 3$. For general N, we have,

$$\begin{aligned} \Pi_{sskf}(\rho) &\equiv B_2^{(N)}(\rho) \equiv \sqrt{\Pi_s(\rho)}, \\ &= \sqrt{\frac{N\,\mathrm{Tr}[\rho^2]-1}{N-1}}. \end{aligned} \tag{36}$$

This is a very interesting property since each was ostensibly derived in different manner.

The picture that has formed seems a natural generalization of the Poincare/Bloch sphere, since the centre of the 8-dimensional hypersphere still represents the totally unpolarized (or maximally mixed) state, and the states on the surface of the hypersphere are totally polarized (pure). There is one essential difference however, that undermines the validity of this picture. In the 2-dimenstional case, all states in or on the Bloch sphere represent valid physical states and a positive density matrix. However, in dimensionality 3 or higher, it has been be shown that the physical constraint of positivity on the polarization matrix restricts the set of valid states to an irrelgular convex region that is a proper subset of the enclosing hypersphere. This physical region touches the surface of the enclosing hypersphere only in some places (where the fully polarized states lie) [23, 24]. That is, many states within the hypersphere and on its surface are unphysical since they would create polarization matrices that are not positive.

The following diagram based on one by Kimura [23] shows all possible 2-dimensional cross sections of the 8-dimensional hypersphere, where the shaded regions represent physical polarization/density matrices. Note that in fact most of the volume inside the hypersphere will be composed of disallowed unphysical states. A state lying on the surface of the hypersphere is a necessary but insufficient condition for it to represent a fully polarized physical state. States anywhere on the border of allowable (shaded) region must have at least one zero eigenvalue. A general state does not necessarily lie on a straight line between the maximally mixed state and a pure state. This must have been the case, since a positive 3×3 matrix in general cannot just be written as a linear combination of the identity matrix (maximally mixed) and a rank 1 matrix (pure), there needs to be a rank 2 component as well. To illustrate these features, let us examine the states represented by points A, B, C and D in fig. (1). These four points are given by the following Bloch vectors:

$$\begin{aligned}\vec{r}_A &= (0,0,0,0,0,0,0,1),\\ \vec{r}_B &= (0,0,0,0,0,0,0,-1),\\ \vec{r}_C &= (0,0,0,0,0,0,0,1/2),\\ \vec{r}_D &= (0,0,\sqrt{3}/8,0,0,0,0,1/8).\end{aligned} \tag{37}$$

Using eq.(31), we can construct the corresponding density matrices, and we find,

$$\rho_A = \begin{bmatrix} 2/3 & 0 & 0 \\ 0 & 2/3 & 0 \\ 0 & 0 & -1/3 \end{bmatrix}, \quad \rho_B = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$
$$\rho_C = \begin{bmatrix} 1/2 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \rho_D = \begin{bmatrix} 1/2 & 0 & 0 \\ 0 & 1/4 & 0 \\ 0 & 0 & 1/4 \end{bmatrix}. \tag{38}$$

We see that ρ_A is not positive, and therefore unphysical, despite lying on the unit hypersphere. This illustrates the breakdown of the analogy with the two-dimensional Bloch sphere addressed above. The matrix ρ_B however is positive therefore physical. Given that it is physical, we can see that it must be a pure state since it lies on the surface of hypersphere, and indeed it is. The matrix ρ_C is also physical, and has a single zero eigenvalue, which is expected since it is at the boundary of allowable states. If it were to move slightly outside the boundary, the zero eigenvalue would become negative and therefore unphysical. The state given by ρ_D is a typical state inside the allowable region.

One may suggest that these properties are a result of an artificial asymmetry of the Gell-Mann matrices (in particular G_3 and G_8), and may be avoided if opt for a different basis set. However, this is not true, and the qualitative properties illustrated above are intrinsic to the $N = 3$ case, and still hold even if one exchanges the Gell-Mann matrices for a different basis set for $SU(3)$ with the same basic properties of Hermiticity, tracelessnesss, and orthogonality. To see this, note that the surface of the hypersphere is 7-dimensional, and that pure states only form a 3-dimensional surface, we realize that, independent of the choice of the basis, the pure states form a very small part of the surface of the generalized Bloch hypersphere. Similar results hold for $N > 3$.

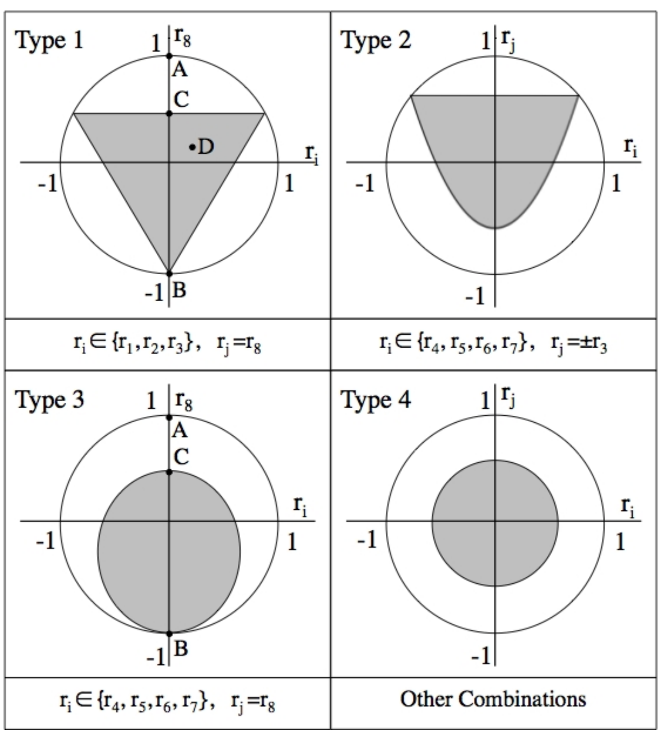

FIG. 1: Classes of cross section of the 8-dimensional space in which the generalized Bloch vectors live, based on diagram by Kimura [23]. In each diagram, the shaded region represents the allowable states, while the outer circle is the enclosing hypersphere. The pure states are where the shaded region touches the outer circle. Points A, B, C, D are specific states we examine.

Yet despite the loss of the simple geometry of a filled hypersphere, the SSKF purity still, in some sense, quantifies the distance of the state from the maximally mixed state. Moreover, as we shall see later, it satisfies the intuitive depolarization criterion for this reason.

IV. COMPARING PURITY MEASURES FOR THREE DIMENSIONS

A. Graphical comparison

Thus far, we have discussed five contending measures of purity for $N = 3$ dimensions: the standard purity Π_s, the von Neumann purity Π_v, Barakat's last measure Π_b, the KW purity Π_{kw}, and the SSKF purity measure Π_{sskf}. Since the standard purity Π_s is just the square of the SSKF purity Π_{sskf}, we ignore the former and only include the latter in our comparison.

To compare the four remaining measures, we set $N = 3$, and recall that the purity will only be a function of the eigenvalues λ_1, λ_2, and $\lambda_3 = 1 - \lambda_1 - \lambda_2$. Therefore, we plot the various measures of purity against λ_2, for various set values of λ_1. After examining the plots, we first note that Π_b, Π_{sskf} and Π_v are always monotonically equivalent in the graphs. That is, they all increase together, decrease together, and have extrema at the same eigenvalues. Put more specifically, derivatives of these three curves always have the same sign. In other words, for any two input states, these three measures always agree which state is more pure.

If functions f and g are monotonically equivalent, we write $f \sim g$. Not that this is an equivalence relation. To rigorously prove that $\Pi_b \sim \Pi_{sskf} \sim \Pi_v$ it suffices to show that each of them is monotonically equivalent to Π_s. It is clear that $\Pi_{sskf} = \sqrt{\Pi_s} \sim \Pi_s$. In the appendix we prove that $\Pi_b \sim \Pi_s$ and $\Pi_v \sim \Pi_s$.

Returning to the graphs, we observe that the KW polarization Π_{kw} often, but not always, gives the opposite results of all the other measures. This suggests that it is measuring something entirely different, and can be better understood through an example.

B. Illustrative example

Recall state C with spectrum $\{1/2, 1/2, 0\}$ and state D with spectrum $\{1/2, 1/4, 1/4\}$. That is their respective density matrices are given by,

$$\rho_C = \begin{bmatrix} 1/2 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad \rho_D = \begin{bmatrix} 1/2 & 0 & 0 \\ 0 & 1/4 & 0 \\ 0 & 0 & 1/4 \end{bmatrix}. \quad (39)$$

Suppose we wish to use one of our measures of purity to find which density matrix ρ_C or ρ_D, is more pure. If we use the measure of purity Π_s or any of the other three in the same monotonic equivalence class, we find

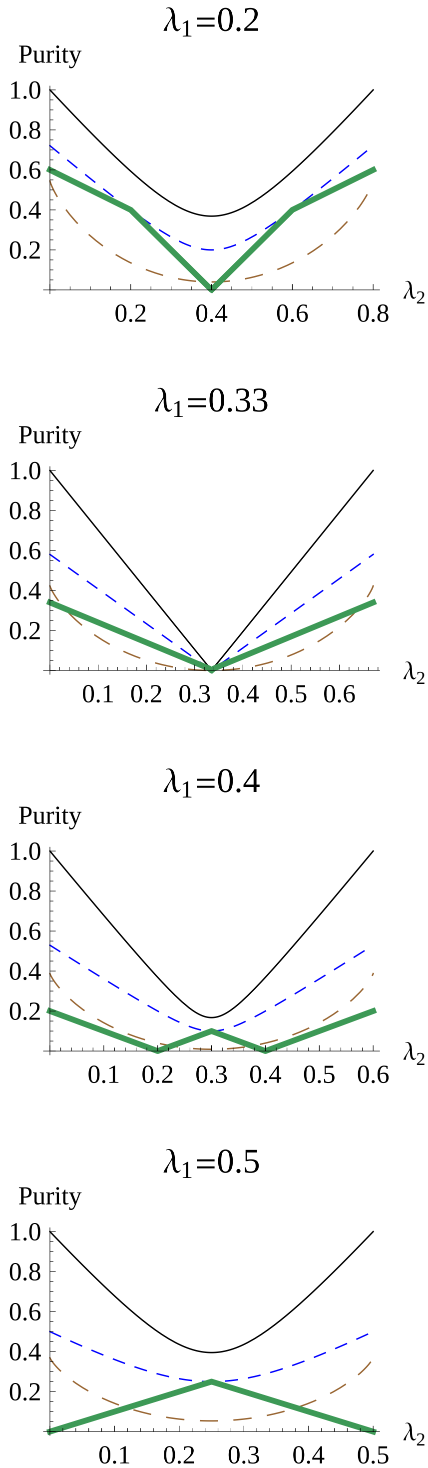

FIG. 2: (Color online) Values of purity measures for various eigenvalues of a three dimensional density matrix. Each graph has fixed λ_1, with λ_2 against the horizontal axis, and $\lambda_3 \equiv 1 - \lambda_1 - \lambda_2$. In each graph, the upper solid curve in black is Barakat's last measure Π_b, the upper dotted curve is the SSKF purity Π_{sskf}, the lower dotted curve is the von Neumann purity Π_v, and the thick solid curve is the KW purity Π_{kw}.

that state ρ_C has higher purity than state D. If we use Π_{kw} we find the opposite, state D is higher in purity. To find out which of these cases is qualitatively expected, we first note that in general, the more mixed a state is, the closer all the eigenvalues are to each other, with the extreme case being the maximally mixed state where all eigenvalues are identical, and the purer a state is the more a small number of eigenvalues should stand out.

We can now reason that each of the density matrices ρ_C and ρ_D have two identical eigenvalues (a "mixed" property), but in ρ_C, the third distinct eigenvalue is further away from the identical two than in ρ_D (that is, $|0-1/2| > |1/2-1/4|$), therefore ρ_C should be more pure. Alternatively, we can reason that since both states have one eigenvalue of $1/2$, then they are equal in this respect, and the other two eigenvalues should be the deciding factor in which state is more pure. The remaining eigenvalues for matrix ρ_D are 0.25, 0.25, these are identical, and for matric ρ_C are 0.5, 0, these are as different as possible. So we expect that ρ_C must have higher overall purity. Therefore any of the measures monotonically equivalent to Π_s, are well-suited for the general idea of overall purity.

However, what if instead of overall purity, we are interested in the component of the density matrix that is completely polarized (i.e. the component that can pass through a three dimensional polarizer unchanged), then we see that,

$$\rho_D = \frac{1}{4}\begin{bmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{bmatrix} + \frac{1}{4}\,\mathbb{I}. \tag{40}$$

That is, ρ_D has a nontrivial fully polarized component, the magnitude of which will be given by $\Pi_{kw}(\rho_D) = 0.25$. The matrix ρ_C however cannot be decomposed in this way, has no fully polarized component that would pass through unchanged through a three dimensional polarizer, and therefore $\Pi_{kw}(\rho_C) = 0$. So we see that which measure of purity is more suitable depends on what we are interested in measuring.

If we are interested in overall purity, we can further narrow down our choice of measure to the SSKF measure of purity Π_{sskf} whenever our systems of interest involve depolarizing channels, a popular type of quantum noise channel. This is shown in the appendix.

C. Relationship between SSKF purity Π_{sskf} and KW purity Π_{kw}

We have already discussed the properties, strengths and weaknesses of Π_{sskf} and Π_{kw}. It is of interest to find a simple relationship between them with aid of a pair of suitably defined variables. The following analysis is similar to results by Sheppard [14]. In the $N = 3$ case there are only 2 degrees of freedom in setting the eigenvalues (since they must sum to unity). We define the following,

$$\begin{aligned} x &\equiv \Pi_{kw} = \lambda_1 - \lambda_2, \\ y &\equiv 3(\lambda_1 + \lambda_2 - 2/3) = 1 - 3\lambda_3. \end{aligned} \tag{41}$$

Physically, x is the KW purity, i.e. the fraction of the power that is in the fully polarized component, and y can be thought of as the fraction power that is not in the completely unpolarized component. In other words, x represents the power in the rank 1 component of the density matrix, while y represents power in the rank 1 or rank 2 components, i.e. the power not in the rank 3. Both x and y vary freely between 0 and 1, with the condition that $y \geq x$ (it follows from $\lambda_2 \geq \lambda_3$). Then we we can express the eigenvalues in terms of x and y,

$$\lambda_1 = \frac{1}{3} + \frac{1}{2}\left(\frac{y}{3} + x\right), \tag{42}$$

$$\lambda_2 = \frac{1}{3} + \frac{1}{2}\left(\frac{y}{3} + x\right), \tag{43}$$

$$\lambda_3 = \frac{1}{3} - \frac{y}{3}. \tag{44}$$

We can make use of these expressions to show that $\lambda_1^2 + \lambda_2^2 + \lambda_3^2 = (2 + 3x^2 + y^2)/6$. Using this result along with eq.(35), Π_{sskf} is expressible as,

$$\Pi_{sskf} = \frac{1}{2}\sqrt{3x^2 + y^2}. \tag{45}$$

This tells us that Π_{sskf} includes the purity from x (i.e. Π_{kw}) plus an additional component from y. Note that for a given x, the minimum value y can take is x, in which case $\Pi_{sskf} = x = \Pi_{kw}$. This is expected, since for y to equal x, this means there is no power in the rank 2 component, and all the polarized power is in the rank 1 component, so both measures agree.

V. RELATION TO ENTAGLEMENT MEASURES

The entanglement of a bipartite system is directly related to the purity of a subsystem once the other subsystem has been traced out. For example, say we have a bipartite system of two qubits, A and B, given by the Bell state,

$$|\Phi\rangle_{AB} = \frac{|00\rangle + |11\rangle}{\sqrt{2}}. \tag{46}$$

This system is maximally entangled. If we define ρ_A as the improper density matrix of the first qubit once the second one has been traced one, we get,

$$\begin{aligned} \rho_A &\equiv \mathrm{Tr}_B\left[|\Phi\rangle\langle\Phi|\right] \\ &= \begin{pmatrix}1/2 & 0\\ 0 & 1/2\end{pmatrix}. \end{aligned} \tag{47}$$

Note that ρ_A is maximally mixed. If we had traced out system A and kept ρ_B it would have been identical. Moreover, if $|\Psi\rangle_{AB}$ where a separable state, then ρ_A would have been a pure rank 1 matrix. So, we see that maximal entanglement leads to maximal mixedness in the subsystem, and no entanglement leads to a pure subsystem state. This argument shows that the mixedness (one minus the purity) of a subsystem is a good measure of entanglement of the whole system.

A common measure of entanglement for a bipartite system is entropy of entanglement E. It is defined as the von Neumann entropy S (i.e. a measure of mixedness) of a subsystem once the other has been partially traced out. That is, it can be written as,

$$E(|\Psi\rangle) = 1 - \Pi_v[\mathrm{Tr}_B(|\Psi\rangle\langle\Psi|)]. \tag{48}$$

What if we replace Π_v in eq.(48) with another measure of purity, say Π_{sskf} or Π_b? This would potentially give rise to another class of entanglement measures with different properties, which could possibly be more relevant for some applications.

For example we consider bipartite systems with $N = 3$, i.e. a system of two qutrits. Such a system has been studied by some authors, and even geometric descriptions developed to help visualize its entanglement [25]. Say we had the following two states,

$$|\Psi_C\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}, \tag{49}$$

$$\begin{aligned} |\Psi_D\rangle &= \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{2}|11\rangle + \frac{1}{2}|22\rangle, \\ &= \frac{\sqrt{2}-1}{2}|00\rangle + \frac{\sqrt{3}}{2}\Big(\frac{|00\rangle + |11\rangle + |22\rangle}{\sqrt{3}}\Big). \end{aligned} \tag{50}$$

If we partially trace out one system in each of these two states, we are left with the subsystem matrices given by eq.(39) in the previous section. Then the we can apply the whole discussion regarding which measures of purity are more suitable, Π_s and its monotonic equivalents, or Π_{kw}. The question of which is more pure, ρ_C or ρ_D, can be asked differently, which is less entangled, $|\Psi_C\rangle$ or $|\Psi_D\rangle$?

In this case, we can further appreciate why Π_{kw} favoured ρ_D as more pure, because it favours $|\Psi_C\rangle$ as more entangled. Note that $|\Psi_C\rangle$ is a two dimensional Bell state in a three dimensional system, and one can think of it in a very specific sense as more entangled than $|\Psi_D\rangle$ since it is equal to a Bell state (even if it is of a lower dimension). One can also reason that $|\Psi_C\rangle$ should have higher entanglement since it has no separable component, whereas $|\Psi_D\rangle$ can be written as a combination of the separable state $|00\rangle$, and the maximally entangled qutrit state.

On the other hand, $|\Psi_D\rangle$ is more entangled than $|\Psi_C\rangle$ (and therefore ρ_C purer than ρ_D), since both have the same coefficient for the $|00\rangle$ state, yet $|\Psi_D\rangle$ has both a $|11\rangle$ and $|22\rangle$ component while $|\Psi_C\rangle$ only has a $|11\rangle$ with no entanglement in the third level whatsoever. Once again, which state is more entangled depends on what exact properties we are looking for.

All of this of course assumes the bipartite state $|\Psi\rangle_{AB}$, is pure. In general, this state can itself be mixed and is written as a density matrix ρ_{AB}, which complicates the situation, and gives rise to the large and growing number of entanglement measures in the literature [26].

VI. CONCLUSION

We showed that quantifying quantum purity for an N level system is equivalent mathematically to quantifying the degree of classical polarization in N dimensions. Then we described and analyzed multiple different measures of purity, finding that which measure is more suitable depends on what we are interested in measuring.

In the more common case of measuring overall purity, we can use either the SSKF purity Π_{sskf}, the von Neumann purity Π_v, Barakat's last measure of purity Π_b, or the standard purity Π_s, all of which are monotonically equivalent. Of these, the measure most consistent with formalisms on quantum channels popular in the quantum computing literature is, Π_{sskf}, given by eq.(33). However, all of these measures are monotonically equivalent, and any of them will suffice for simple comparison of purity between states. The standard purity Π_s in particular is the simplest to use and the most common in the quantum mechanics literature.

If instead we are interested only in the component that is fully polarized, then the KW purity Π_{kw} is a more suitable measure, and will yield the strength of only the fully polarized part, discarding other components. It can be shown that for $N = 3$, Π_{sskf} and Π_{kw} are related in a simple manner once we add a variable to represent the second degree of freedom.

Moreover, there is a direct relationship between the entanglement of a pure bipartite state and the purity of one of its subsystems once the other subsystem has been traced out. This can be used to give insight into measures of entanglement, and possibly create new entanglement measures based on various measures of purity.

Appendix A: Gell-Mann matrices

The Gell-Mann matrices ($G_i, i = 1, ..., 8$) are a popular set of generators for the special unitary group $SU(3)$ [22].

They are given by,

$$G_1=\begin{bmatrix}0&1&0\\1&0&0\\0&0&0\end{bmatrix}, \qquad G_2=\begin{bmatrix}0&-i&0\\i&0&0\\0&0&0\end{bmatrix},$$
$$G_3=\begin{bmatrix}1&0&0\\0&-1&0\\0&0&0\end{bmatrix}, \qquad G_4=\begin{bmatrix}0&0&1\\0&0&0\\1&0&0\end{bmatrix},$$
$$G_5=\begin{bmatrix}0&0&-i\\0&0&0\\i&0&0\end{bmatrix}, \qquad G_6=\begin{bmatrix}0&0&0\\0&0&1\\0&1&0\end{bmatrix},$$
$$G_7=\begin{bmatrix}0&0&0\\0&0&-i\\0&i&0\end{bmatrix}, \qquad G_8=\frac{1}{\sqrt{3}}\begin{bmatrix}1&0&0\\0&1&0\\0&0&-2\end{bmatrix},$$

They are all Hermitian, traceless, and satisfy the orthogonality relation $\mathrm{Tr}\left[G_iG_j\right]=2\delta_{ij}$, where δ_{ij} is the Kronecker delta.

Appendix B: Monotonic equivalence of Π_b and Π_v to Π_s

Assume we have an N dimensional state, with eigenvalues $\lambda_1,...,\lambda_N$, with the first $N-1$ eigenvalues independent, and λ_N satisfying,

$$\lambda_N = 1-\sum_{j=1}^{N-1}\lambda_j. \tag{1}$$

Then by eq.(11), eq.(14), and eq.(28),

$$\Pi_s = \sum\lambda_j^2 + (1-\sum\lambda_j)^2, \tag{2}$$
$$\Pi_v = 1+\frac{\sum\lambda_j\log_2\lambda_j + (1-\sum\lambda_j)\log_2(1-\sum\lambda_j)}{\log_2 N}, \tag{3}$$
$$\Pi_b^2 = 1-N^N\lambda_1\lambda_2...\lambda_{N-1}(1-\sum\lambda_j), \tag{4}$$

where all sums over j in this section run from 1 to $N-1$. We have squared Π_b since it does not affect monotic equivalence, and makes the calculation more tractable. The three expressions above monotonically equivalent if $\frac{\partial\Pi_s}{\partial\lambda_i}$, $\frac{\partial\Pi_v}{\partial\lambda_i}$, and $\frac{\partial\Pi_b^2}{\partial\lambda_i}$ have the same sign for each $i=1,2,...,N-1$. We have,

$$\begin{aligned}\frac{\partial\Pi_s}{\partial\lambda_i} &= 2\lambda_i - 2(1-\sum\lambda_j)\\ &= 2\lambda_i - 2\lambda_N\end{aligned} \tag{5}$$
$$\begin{aligned}\frac{\partial\Pi_v}{\partial\lambda_i} &= \frac{1}{\log_2 N}[\log_2\lambda_i - \log_2(1-\sum\lambda_j)],\\ &= \frac{1}{\log_2 N}[\log_2\lambda_i - \log_2\lambda_i]\end{aligned} \tag{6}$$
$$\begin{aligned}\frac{\partial\Pi_b^2}{\partial\lambda_i} &= -N^N\lambda_1...\lambda_{i-1}\lambda_{i+1}...\lambda_{N-1}(1-\sum\lambda_j-\lambda_i),\\ &= N^N\lambda_1...\lambda_{i-1}\lambda_{i+1}...\lambda_{N-1}(\lambda_i-\lambda_N).\end{aligned} \tag{7}$$

We see that $\frac{\partial\Pi_s}{\partial\lambda_i}$ and $\frac{\partial\Pi_b^2}{\partial\lambda_i}$ both equal a positive number multipled by $\lambda_i-\lambda_N$, and therefore will have the same sign. Also note that $\lambda_i-\lambda_N$ will always have the same sign as $\log_2\lambda_i-\log_2\lambda_N$, since $\lambda_i>\lambda_N \iff \log_2\lambda_i > \log_2\lambda_N$. Therefore the three measures Π_s, Π_v and Π_b are monotically equivalent, and will always give the same result if one uses them to find out which of two quantum states is more pure.

Appendix C: Depolarizing channels as a criteria

Consider a depolarizing channel, an important type of quantum noise [6]. It is a transformation which *depolarizes* the input quantum state with probability p, (i.e. replaces it with $\mathbb{I}/N$), and leaves it unchanged with probability $1-p$. This channel is given by the following superoperator,

$$\mathcal{E}(\rho) = p\frac{\mathbb{I}}{N} + (1-p)\rho. \tag{1}$$

Applying the SSKF polarization measure of purity in eq.(36) to the output of this channel, we find,

$$\Pi_{sskf}(\mathcal{E}(\rho)) = (1-p)\Pi_{sskf}(\rho). \tag{2}$$

We observe that eq.(2) has a very simple and intuitive form, showing that the purity simply scales down by a factor of $(1-p)$ after the state passes through the depolarizing channel. This intuitive relationship does not hold for other measure of purity, even ones that are monotonically equivalent to Π_{sskf}. This suggests Π_p is a measure with more physical meaning, and more relevant whenever depolarizing channels are in effect, as they often are.

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